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COMPUTED HEATS OF FORMATION OF THREE DIAZAPENTALENES, AND TWO *GEM*-DINITRO/*GEM*-DIFLUORAMINO ANALOGUES OF RDX

by

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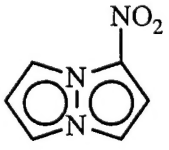
13. ABSTRACT (Maximum 200 words)

Computed heats of formation for **1** - **5**.



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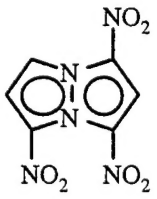

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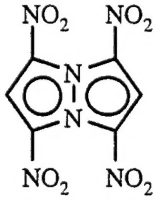

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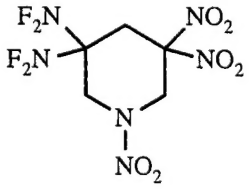

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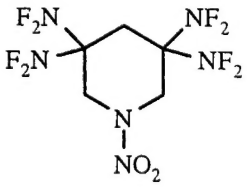

5

1: ΔH_f^{298K} (solid) = 61 kcal/mole = 402 cal/g

2: ΔH_f^{298K} (solid) = 67 kcal/mole = 276 cal/g

3: ΔH_f^{298K} (solid) = 78 kcal/mole = 273 cal/g

4: ΔH_f^{298K} (solid) = –51 kcal/mole = –160 cal/g

5: ΔH_f^{298K} (solid) = –77 kcal/mole = –230 cal/g

14. SUBJECT TERMS	15. NUMBER OF PAGES
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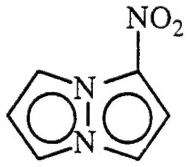
We have used our density functional procedure [1] to compute the heats of formation of the compounds **1** - **5**. **1** and **2** have been prepared by R. Schmitt and J. Bottaro at SRI and **3** is under consideration. The syntheses of **4** and **5** are being pursued by T. Axenrod (CUNY). The vibrational energies were determined from the molecular stoichiometries [2]. The density functional calculations give the gas phase heat of formation, which we convert to the solid state value by subtracting the heat of sublimation. The latter is obtained by means of the relationship that we have developed between the heat of sublimation and the computed electrostatic potential on the molecular surface [3].

Results:

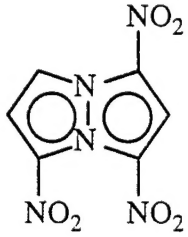
1



ΔH_f^{298K} (gas) = 84 kcal/mole = 553 cal/g

ΔH_f^{298K} (solid) = 61 kcal/mole = 402 cal/g

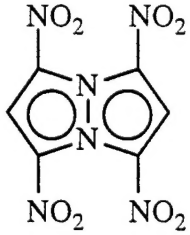
2



ΔH_f^{298K} (gas) = 97 kcal/mole = 401 cal/g

ΔH_f^{298K} (solid) = 67 kcal/mole = 276 cal/g

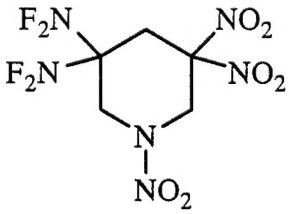
3



ΔH_f^{298K} (gas) = 113 kcal/mole = 394 cal/g

ΔH_f^{298K} (solid) = 78 kcal/mole = 273 cal/g

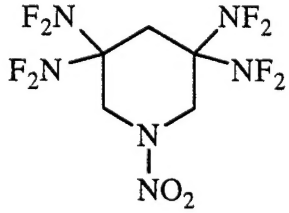
4



ΔH_f^{298K} (gas) = –13 kcal/mole = –42 cal/g

ΔH_f^{298K} (solid) = –51 kcal/mole = –160 cal/g

5



ΔH_f^{298K} (gas) = –40 kcal/mole = –120 cal/g

ΔH_f^{298K} (solid) = –77 kcal/mole = –230 cal/g

For comparison, the experimental gas phase ΔH_f^{298K} value for RDX is 206 cal/g [4,5].

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